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High-Fidelity Geometric Modeling and Mesh Generation for Mechanics Characterization of Polycrystalline Materials

**Grant/Contract Number**
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**The full name of the principal investigator on the grant or contract.**

Yongjie Zhang

**Program Manager**
**The AFOSR Program Manager currently assigned to the award**

Fariba Fahroo and David Stargel

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10/01/2011

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09/30/2014

**Abstract**

During the Fiscal Year 2014 (from October 1, 2013 to September 30, 2014), the PI and her group worked on the following three problems. Based on our research, we have published four book/book chapters [1-4], 7 peer-reviewed journal papers [5-11] and 2 peer-reviewed conference papers [12-13].

(1) Image Restoration of Phase Contrast Nano Scale X-ray CT Images
Zernike phase contrast is a useful technique for nanoscale X-ray computed tomography (CT) of materials with a low X-ray absorption coefficient. It enhances the image contrast using a phase ring. However, it also creates artifacts that hinder the use of traditional image segmentation techniques. We have developed an image restoration method [5] that models the X-ray phase contrast optics, computes a 3D kernel and minimizes an energy function. Though similar ideas have been used for visible light microscopy, this method employs an effective edge detection method and can be applied on various types of samples. Using this algorithm, we restore multiple phase contrast X-ray CT images and threshold them to produce segmented results. We quantitatively evaluate and compare our method to other segmentation techniques to demonstrate its high accuracy.

(2) Extended Edge-Weighted Centroidal Voronoi Tessellation for Image Segmentation
We have extended the basic edge-weighted centroidal Voronoi tessellation (EWCVT) for image segmentation to a new advanced model [6], namely harmonic edge-weighted centroidal Voronoi tessellation (HEWCVT). This extended model introduces a harmonic form of clustering energy by combining the image intensity with cluster boundary information. Improving upon the classic CVT and EWCVT methods, the HEWCVT algorithm can not only overcome the sensitivity to the seed point initialization and noise, but also improve the accuracy and stability of clustering results, as verified in several types of images. We then present an adaptive superpixel generation algorithm based on HEWCVT. First, an innovative initial seed sampling method based on quadtree decomposition is introduced, and the image is divided into small adaptive segments according to a density function. Then, the local HEWCVT algorithm is applied to generate adaptive superpixels. The presented algorithm is capable of generating adaptive superpixels while preserving local image features efficiently.

(3) Adaptive and Anisotropic Surface T-mesh Generation from Cross Field
In this study, an extended cross field-based parameterization method [7, 12] is developed to adapt the parametric line spacings to different surface resolutions. Moreover, an anisotropy defined from an input scalar field can also be achieved. From the parameterization results, we extract adaptive and anisotropic T-meshes for the further T-spline surface construction. Finally, a gradient flow-based method is developed to improve the T-mesh quality, with the anisotropy preserved in the quadrilateral elements. The effectiveness of the presented algorithm has been verified using several complex models.

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**Archival Publications (published) during reporting period:**

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**14. ABSTRACT**
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1. Image-Based Geometric Modeling and Mesh Generation.
2. Quality Improvement for Segmented Hexahedral Meshes Using Geometric Flows.
3. Adaptive and Anisotropic All-Hexahedral Mesh Generation Using a Hybrid Octree and Bubble Packing.
4. Octree-based Dual Contouring Method for Triangular and Tetrahedral Mesh Generation with Guaranteed Angle Range.

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**Contract/Grant Title:** High-Fidelity Geometric Modeling and Mesh Generation for Mechanics Characterization of Polycrystalline Materials
**Contract/Grant #:** FA9550-11-1-0346
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**Annual accomplishments (200 words max):**

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2. **Extended Edge-Weighted Centroidal Voronoi Tessellation for Image Segmentation.** We have developed an extended model [6] named harmonic edge-weighted centroidal Voroni tessellation. This method can overcome the sensitivity to the seed point initialization and noise, and also improve the accuracy and stability of clustering results,
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**Changes in research objectives, if any:** None
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## Abstracts (250 words or more)

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In this study, an extended cross field-based parameterization method [7, 12] is developed to adapt the parametric line spacings to different surface resolutions. Moreover, an anisotropy defined from an input scalar field can also be achieved. From the parameterization results, we extract adaptive and anisotropic T-meshes for the further T-spline surface construction. Finally, a gradient flow-based method is developed to improve the T-mesh quality, with the anisotropy preserved in the quadrilateral elements. The effectiveness of the presented algorithm has been verified using several complex models.

## Research Progress

This section will describe the accomplishments in detail for Fiscal Year 2014 for the project. The PI and her group mainly worked on three specific problems.

**1. Image Restoration of Phase Contrast Nano Scale X-ray CT Images**

X-ray CT images can be very effective in differentiating materials by their density and absorption coefficient. However, many materials in engineering applications, such as polymers, carbon structures and soft tissues, often have a low atomic number and offer negligible contrast relative to their surroundings. In addition, many of these materials have sub-micron features of interest that require nanoscale resolution X-ray CT (nanoCT). The use of lens-based X-ray optics, that achieves resolutions as high as 30-50nm, makes Zernike phase contrast the most suitable technique for nanoCT. Unfortunately, this imaging technique produces an image with artifacts, which makes image segmentation a significant challenge. The two main artifacts are halos and shade-off. Halos are bright or dark thin regions around the boundary of the sample. These false edges around the object make many segmentation algorithms, such as level-set and region growing methods, less robust. Shade-off refers to the similar range of intensities the object and the background share away from edges. This reduces the efficiency of methods based on histogram analysis. Due to these artifacts, standard segmentation techniques produce inaccurate results despite structural boundaries being clearly visible to the human eye.

Efforts to automate the segmentation of phase contrast images have mostly been applied in visible light biological microscopy. It is still a developing area of research. There is no general optimal method and post hoc methods are often applied. Morphology tools and Laplace of Gaussian filters for edge detection are prone to errors due to shade-off. Level set methods tend to fail at halos and boundaries with large gradients. However, they can be improved using machine learning-based validations and intelligent contour initialization. Restoring artifact-free images based on a derived model of the microscope optics can also make segmentation more robust. Current trends show that the use of phase contrast imaging is becoming more prevalent in X-ray microscopy. The primary research focus has been on developing new reconstruction methods to improve the quality and increase the contrast of CT images. Previous work retrieved the phase shift of each radiograph by modelling the refractive index of the object. Other interesting methods include frequency harmonics, regularization techniques and optics modeling. However, a lot of these attempts verified their theoretical work using simulations and have not focused on segmenting acquired CT images.

Lastly and importantly, phase retrieval algorithms often perform poorly for Zernike phase contrast, leaving a dearth of previous work for this application. Fig. 1(a) shows the important components of a typical nanoCT instrument using Zernike phase contrast optics. The Fresnel zone plate (FZP) achieves the nanoCT's high resolution by means of diffraction. Upon transmission through the sample, the waveform from the X-ray source can be divided into two different components, the diffracted and undiffracted waves. As shown in Fig. 1(b), the phase difference between the diffracted wave and sample wave, which is the sum of all waves, is related to the change in refractive indices of the wave medium. However, the resulting amplitude difference is minimal and provides insufficient image contrast. The key component of Zernike phase contrast is the phase ring. It increases the image contrast by phase shifting the undiffracted waved by $-\pi/2$. However, a fraction of the diffracted wave leaks onto the phase ring and is also phase shifted by $-\pi/2$. As a result, bright artifacts appear where the magnitude of the sample wave is lower than that of the undiffracted wave. This is illustrated in Fig. 1(c).

Our work aims to deconvolve nanoCT images, eliminate the artifacts and generate accurate segmented results. To that end, we model the phase contrast optics of a nanoCT instrument, minimize an energy function and threshold the restored images. We present the modelling of the nanoCT components and the computational tools to derive the system's kernel. It also outlines our method of computing the 3D kernel, which allows us to extend our method to CT images from radiographs. The set up of an inverse problem is a new technique for Zernike phase contrast in nanoCT. An energy function and the robust edge detection method are used to solve the inverse problem. This solution procedure is more flexible for samples with different geometries than that of previous restoration technqiues in visible light microscopy. We use multiple CT images obtained from the nanoCT (UltraXRM-L200, Xradia Inc., Pleasanton, CA) for testing and show their restored images and segmentations. Despite ground truth segmentations not available, we qualitatively and quantitatively show the high accuracy of our results. Figure 2 shows an example.

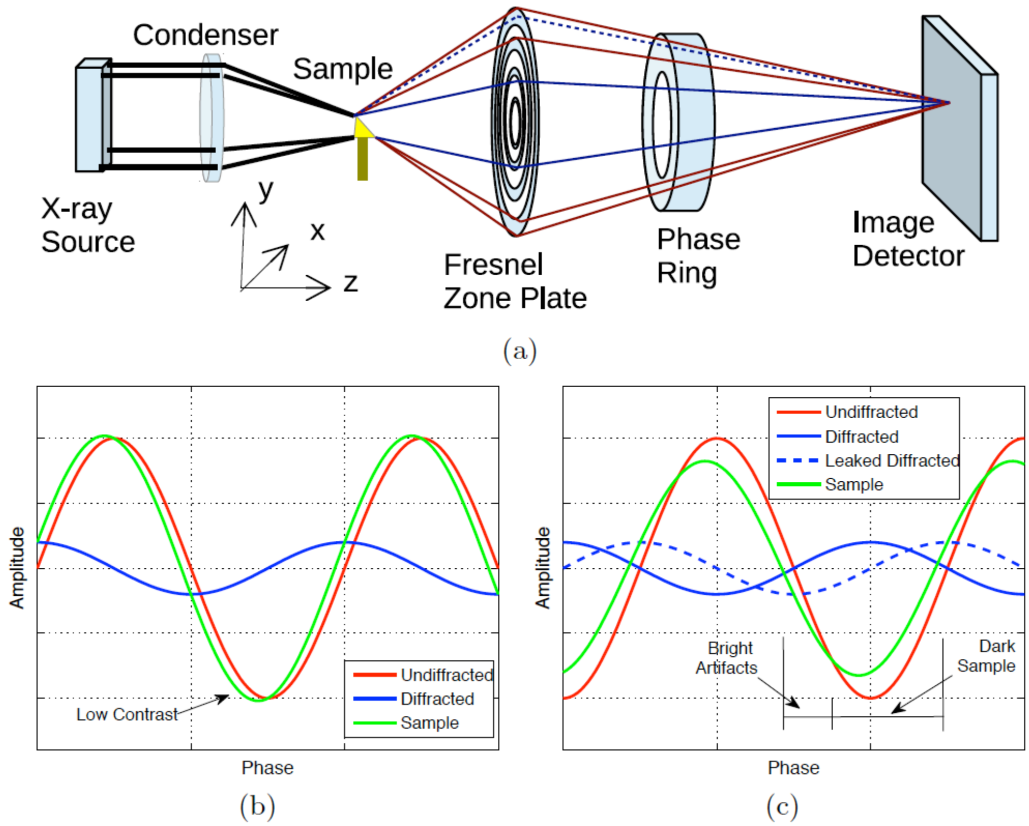



**Figure 1.** Illustration of the benegits and drawbacks of the phase ring. (a) Schematic of the diffracted and undiffracted waves through the important components of a CT machine; (b) low contrast without the phase ring; and (c) higher contrast and artifacts due to the negative shift of the undiffracted wave and a portion of the diffracted wave respectively.

## 2. Extended Edge-Weighted Centroidal Voronoi Tessellation for Image Segmentation

Image segmentation has been one of the core topics in computer vision and image processing for decades. Its central task is to partition an image into subsets of pixels that share similar characteristics, such as color, brightness or texture. The success of most tasks requiring image analysis is often a direct consequence of the success of segmentation. Many methods have been developed for image segmentation, such as thresholding, edge detection, level set method and clustering techniques. Since each method has its own advantages and drawbacks, the appropriate method tends to depend on the nature of the particular application. As an over-segmentation of the image, superpixels have also become popular as they provide an efficient preprocessing tool for various computer vision applications. A superpixel is defined as a homogeneous image region that aligns well with object boundaries. It has been shown that using superpixels is advantageous because they can preserve natural image boundaries and reduce redundant information of the image data as well as enforce local consistency. Many algorithms have been developed to divide an image into superpixels, such as NCuts, TurboPixel and SLIC.

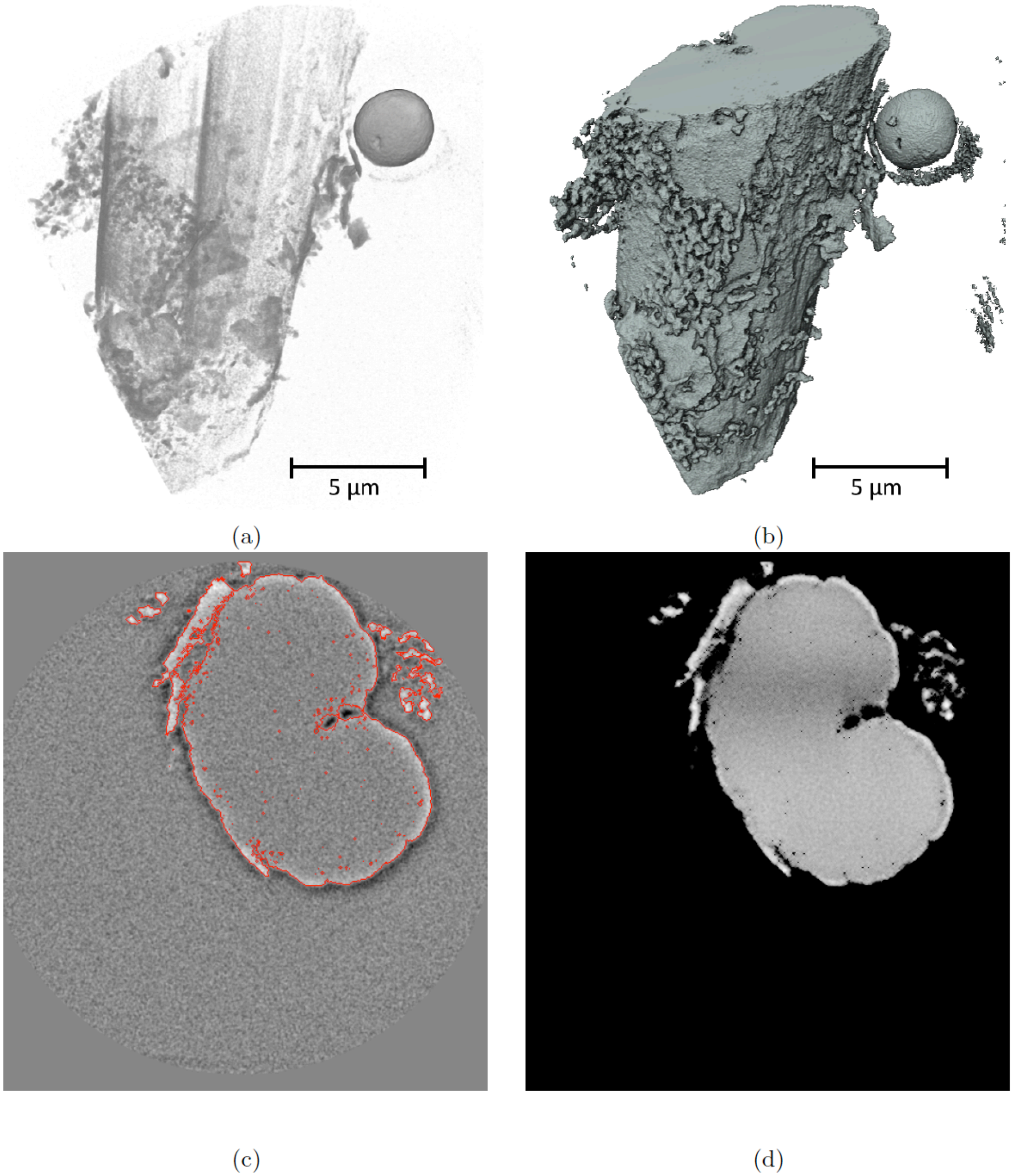
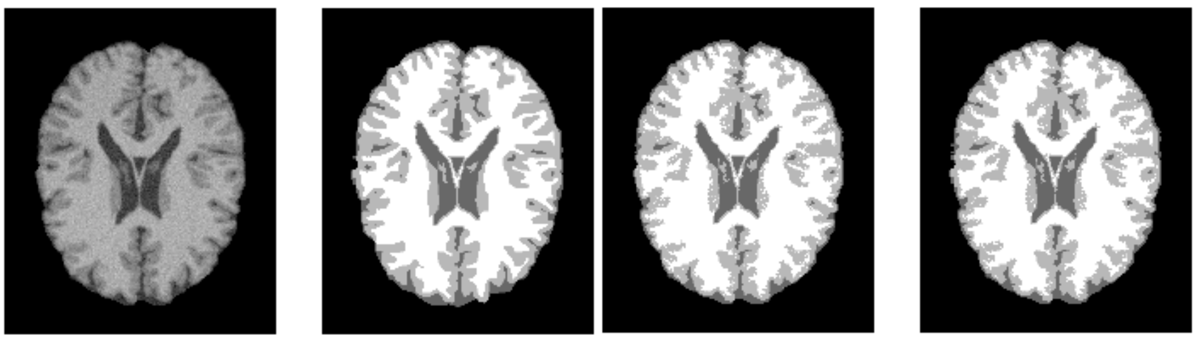
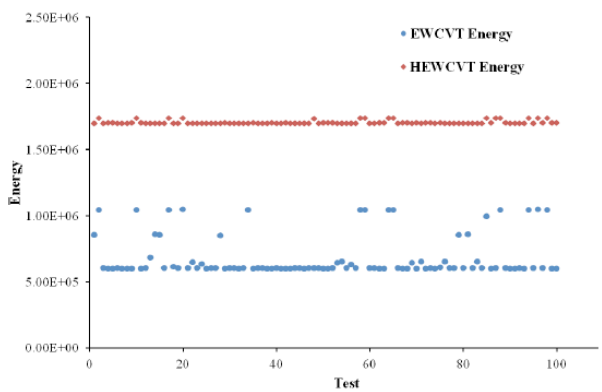



**Figure 2.** Volume rendering of the (a) high intensities and (b) segmentation of the fiber coated with PTFE. A slice of the (c) original image, whose segmentation is outlined by the red curve, and (d) corresponding slice of the original image.

In recent years, a lot of efforts have been put into the research of Centroidal Voronoi tessellation (CVT) based methods for both image segmentation and superpixel generation. The classic CVT method and edge-weighted centroidal Voronoi tessellation (EWCVT) methods are sensitive to seed point initialization, which may result in incorrect and unstable segmentation results. To extend the EWCVT method for both image segmentation and superpixel generation, we first develop an innovative model named harmonic edge-weighted centroidal Voronoi tessellation (HEWCVT) for image segmentation. The proposed method extends and improves upon the EWCVT method by using the harmonic formulation in the clustering energy function. We then present an adaptive superpixel generation algorithm based on the local HEWCVT. Compared to the classic CVT and EWCVT methods, our proposed algorithms have three main advantages: (1) our HEWCVT-based segmentation scheme is much more stable and less sensitive to the initializations due to an imposition of a soft membership onto the data points; (2) the segmentation accuracy is also improved since the spatial information of local image features is integrated into the harmonic form energy function to compensate for the effect of noise; and (3) we propose an innovative adaptive superpixel generation algorithm using quadtree decomposition and density function, yielding high quality adaptive superpixels with image features preserved efficiently. Figures 3-4 show two examples.



(a) Original image (b) Ground truth (c) EWCVT (d) HEWCVT




(e) Energy outputs

**Figure 3.** Segmentation results of a brain MRI-T1 image with 7% noise and 20% INU. (a) Original image; (b) ground truth result; (c) EWCVT; (d) HEWCVT; and (e) energy outputs.

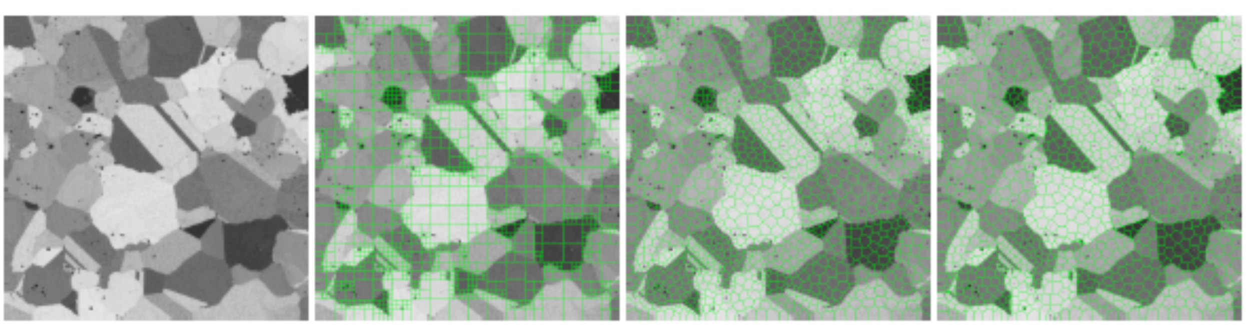


**Figure 4.** Adaptive superpixel generation results of Alloy. From left to right: original image, quadtree decomposition, CVT in physical space, and adaptive superpixels.

### 3. Adaptive and Anisotropic Surface T-mesh Generation from Cross Field

T-mesh is made up of quadrilateral elements with T-junctions on the edges. In recent years, global parameterization methods were introduced to generate quadrilateral meshes. Some of these methods capture surface features using a cross field, and align the quadrilateral elements to the feature directions. Most of the methods yield uniform quadrilateral elements. It remains a challenge to achieve the adaptation or anisotropy together with the orthogonality in the parametric lines due to the difficulty in the vector field optimization. In this study, we extended the cross field-based method for adaptive and anisotropic parameterization, which adapts the parametric line spacings to multi-resolution surface features; and also developed a new gradient flow-based method for T-mesh quality improvement, with the anisotropy in quadrilateral elements preserved. Figure 5 shows three results.

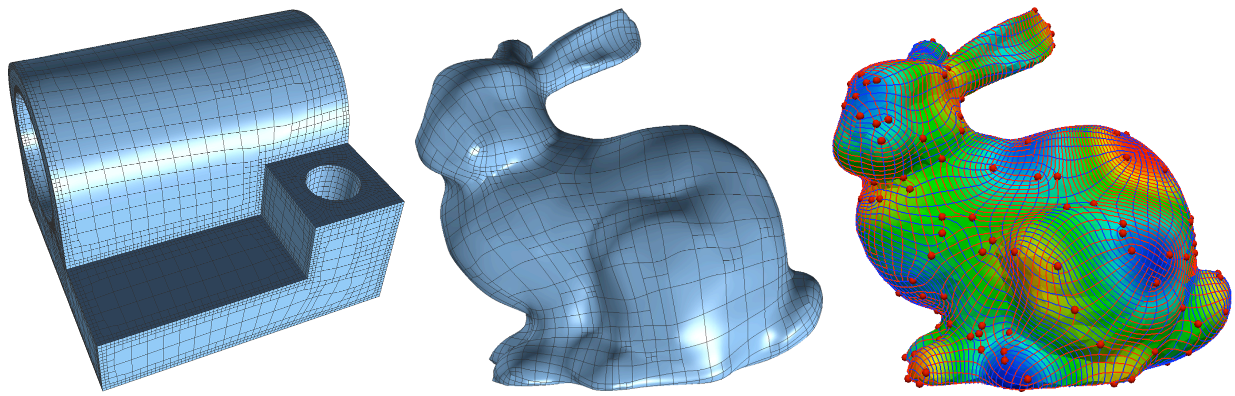


**Figure 5.** Isotropic (left and middle) and anisotropic (right) T-mesh results of a bunny model. For the right picture, one eigenfunction is used to build the cross field.

## Conclusion

During FY 2014, the PI and her group worked on three specific research problems: (1) Image Restoration of Phase Contrast Nano Scale X-ray CT Images; (2) Extended Edge-Weighted Centroidal Voronoi Tessellation for Image Segmentation; and (3) Adaptive and Anisotropic Surface T-mesh Generation from Cross Field. Based on our research, we have published four book/book chapters [1-4], 7 peer-reviewed journal papers [5-11] and 2 peer-reviewed conference papers [12-13].

## References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